# Lattice QCD with open boundary conditions

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**Based on work done in collaboration with Martin Lüscher**

# Problem

## Rising cost as $a \to 0$

- Need more points for fixed volume $L =$const $\to N = L^4 a^{-4}$.
- Monte Carlo time scales as $a^{-2}$.
- Topological sectors emerge $\to$ simulation gets stuck
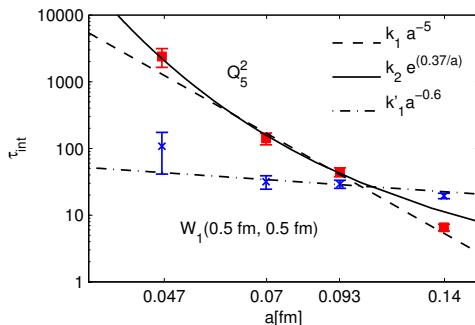
## Solutions

- Fix topological sector.
    - Loss of unitarity.
    - Deal with $1/V$ corrections.
- Open the lattice.

# Scaling in pure gauge theory

- Topological charge shows dramatic slow down: periodic b.c.
- Pure gauge theory

SOMMER, VIROTTA, ST.S'10

# Topological Charge

## Slowing down

- Topological sectors emerge in continuum limit.
- Simulation gets stuck.

## Fermions

- Some folklore that fermions solve the problem.
- Distribution of $Q$ gets narrower at light quark mass.
- Different effective gluonic action
  $\rightarrow$ influences coefficient.
- Slow topology observed, e.g., by MILC, ALPHA.
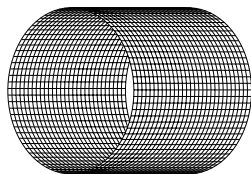
# Open boundary conditions

## Proposed solution

- open boundary condition in time direction
  → same transfer matrix, same particle spectrum
- periodic boundary condition in spatial directions
  → momentum projection possible
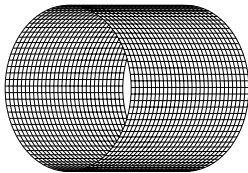
# Open boundary conditions



- Periodic boundary conditions in space.
- Neumann boundary conditions in time.

- Gauge fields

$$F_{0k}|_{x_0=0} = F_{0k}|_{x_0=T} = 0, \quad k = 1, 2, 3$$

- Fermion fields

$$P_+\psi(x)|_{x_0=0} = P_-\psi(x)|_{x_0=T} = 0 \qquad P_\pm = \frac{1}{2}(1 \pm \gamma_0)$$

$$\bar{\psi}(x)P_-|_{x_0=0} = \bar{\psi}(x)P_+|_{x_0=T} = 0$$

# On shell improvement

## Boundary terms

### Gauge action

$$\delta S_{G,b} = \frac{1}{2g_0^2}(c_G - 1) \sum_{p_s} \text{tr}(1 - U(p_s))$$
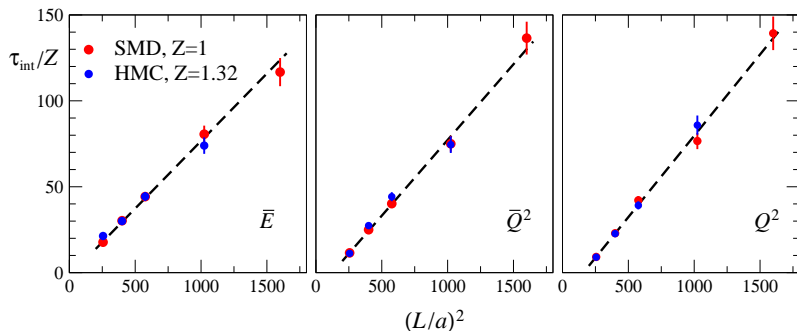
### Fermion action

$$\delta S_{F,b} = a^3(c_F - 1) \sum_{\vec{x}} \left( \bar{\psi}(x)\psi(x)|_{x_0=a} + \bar{\psi}(x)\psi(x)|_{x_0=T-a} \right)$$

- Very similar to Schrödinger functional.
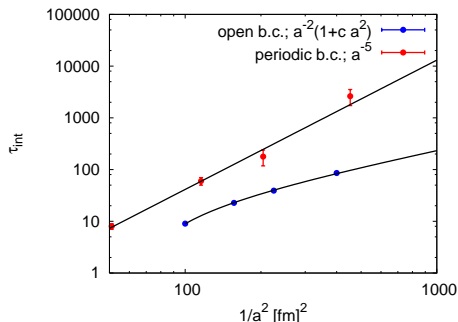- If one stays clear of boundaries, might not be needed.

# Pure gauge theory: $\tau_{\text{int}}$ vs $a^{-2}$

M. Lüscher, St.S, JHEP 1107 (2011) 036



- $L =$ const
- scaling linear in $a^{-2}$.
- no effect of sector forming visible.

# Pure gauge theory: Periodic vs Open boundaries



- Open boundary conditions solve problem.
- Scaling of the topological charge same as other observables.
- Already at typical $a$ sizable improvement.

# Large T

## Finite volume

- For $T \to \infty$ the effect of the b.c. vanishes.
- But also the effect on observables vanishes as $V^{-1}$.

## Dependence on $T$

- Width of distribution of $Q$ is $\propto \sqrt{TL^3}$.
- Change of charge through boundary $\propto \sqrt{L^3}$.
  $\to$ expect $\tau_{\text{int}} \propto T$, for random walk
- For each $T$, there is an $a$ from which the boundary tunneling dominates over the bulk tunneling.

# Analysis

- Physics in the center as with period. bound. cond.
- Boundary effects decay with lightest state of vaccuum quantum numbers. $\rightarrow 2\pi$
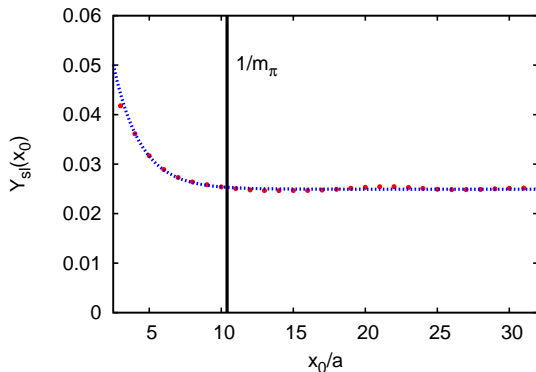- How is the effect in actual simulations?

# Setup
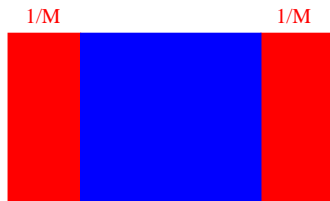
## Action

- $N_{\mathrm{f}} = 2 + 1$ NP improved Wilson fermions
- Iwasaki gauge action
- $64 \times 32^3$ lattice with $a = 0.09$fm
- studied extensively by PACS-CS
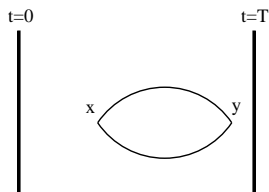- $m_\pi = 200$MeV; $m_\pi L = 3$

## Reweighting

- Simulate fermion action with spectral gap.
- Include reweighting factor in measurement.
- Stabil simulation, no ergodicity problems.

# Yang-Mills action density



- Gauge action density from smoothed links.
- Boundary effects decay with mass $\approx$ 1GeV.
- $m_\pi \approx$ 200MeV.

# Boundary conditions



$$C(x_0, y_0) = \sum_{\mathbf{x}, \mathbf{y}} \langle P(x_0, \mathbf{x}) P(y_0, \mathbf{y}) \rangle$$
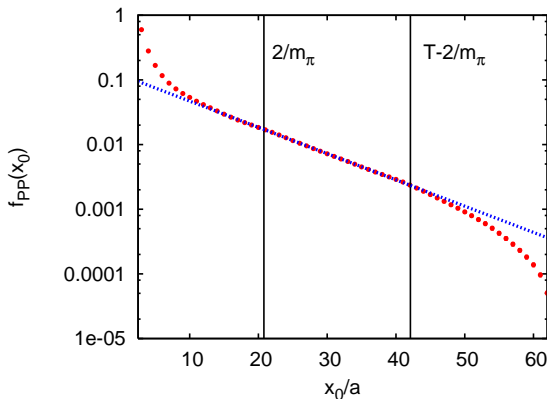
- Source point $y$, zero momentum projection
- With periodic bc get $\cosh(m(x_0 - y_0))$ behavior

## Open boundary conditions

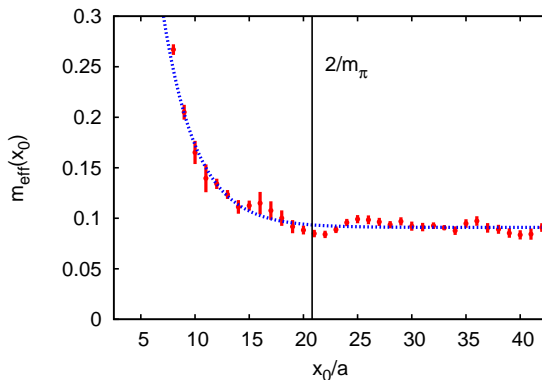Dirichlet boundary condtions for hadron propagator

$$C(x, y) \propto \sinh(m(T - x_0)) \qquad \text{for} \quad x_0 > y_0$$
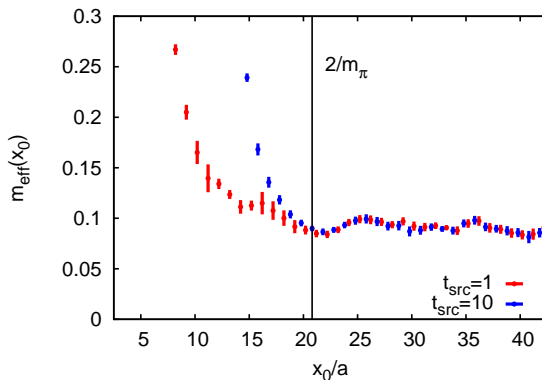
# Pseudoscalar Correlator



- source at $y_0/a = 1$
- exponential fall-off $2/m_\pi$ away from source/boundary

# Pseudoscalar Correlator: effective mass



- Mass agrees with PACS-CS (interpolated) value

# Effect of the position of the source



- Source on boundary couples strongy to excited states
- Plateau starts about at same time slice.

# Conclusions

- Simulations with reduced rate of tunneling cannot produce accurate results.
- Open boundary conditions **in time** solve the problem of frozen topology.
- Fermion simulations without particular problems.
- Measurements $2/m_\pi$ from boundary.
- Reweighting makes Wilson simulations safe.